

Improvement of Single- and Multicore Performance of Compressible and Incompressible Flow Solver Within the BoSSS Framework

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Clusters
Lichtenberg Cluster Darmstadt

Software
BoSSS

Additional Software
Intel math kernel library (MKL), METIS

Institute
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Introduction

Within the past decade, discontinuous Galerkin (DG) methods have attracted significant interest in a broad range of computational sciences such as computational electromagnetics, computational astrophysics and fluid dynamics (CFD). A major advantage of DG methods is their high accuracy in comparison to methods, which are currently used in industry (finite volume and finite element methods, FVM resp. FEM). Furthermore, DG methods are also much better suited for future high performance computer architectures.

Until now, the DG solver framework BoSSS, which is under active development at the Chair of Fluid dynamics (FDY), has only been validated for small physical two dimensional flow test cases. Amongst others the BoSSS framework shall be capable of simulating turbulence. Typical physical properties of turbulence can only be investigated in three dimensional simulations. Due to increase in degrees of freedom, especially in combination with higher DG methods, three dimensional simulations are very extensive. To master this challenge, the scalability of the current code, which is parallelized by using the MPI standard, has to be investigated and improved. Additionally, benchmarking has to be made for solving large sparse non-linear systems with parallel direct or iterative solvers.

Methods

The following solvers of the BoSSS framework are investigated in this project:

- compressible Navier-Stokes (CNS) Solver: artificial viscosity, local time stepping scheme (explicit), testcase: double mach reflection
- extended discontinuous galerkin (XDG) Solver: symmetric interior penalty, XDG approach, testcase: Poisson-Problem

The solvers are investigated to identify bottlenecks, which constrain scalability. The message passing interface (MPI) standard is used for parallelization of these solvers. Due to the DG approach and explicit time stepping the CNS solver is easier to parallelize in comparison to implicit time stepping, which requires to solve an equation system. So in the context of MPI bad communication and load balancing are the likely bottlenecks of the CNS solver. The XDG discretization of the Poisson problem leads to a sparse linear equations system and can be seen as a minimal example of a XDG discretization. The sparse linear system is solved by Krylov-subspace methods in combination with different experimental preconditioners.² This project is used to investigate the scalability of these methods and to define optimization potential. The optimization of linear solvers is the base for further performance improvement of the incompressible flow solver in the BoSSS framework. Both solvers partly rely on libraries such as the Intel math kernel library (MKL)³ or the graph partitioning algorithm METIS.⁴ On Unix-like operating systems there are many libraries available. To test, which library suits the best for the solver is also a target of this project. As a side product the portability of the framework is investigated, which is originally developed in C# on Windows-based systems.

Results

The following results were achieved:

- experimental linear solver tested (unpublished content, details spared)
- portability to unix-based systems improved, work of M.Rieckmann
- several benchmark runs of CNS solver completed on the Lichtenberg Supercomputer

Publications

Geisenhofer, M.; Kummer, F.; Müller, B.: A discontinuous Galerkin immersed boundary solver for compressible flows: Adaptive local time stepping for artificial viscosity-based shock-capturing on cut cells. International Journal for Numerical Methods in Fluids, 2019
<https://doi.org/10.1002/flid.4761>

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